

## Electron impact excitation of the $np^5nd$ and $np^5(n+2)s$ states of Ar( $n=3$ ) and Xe( $n=5$ ) atoms

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**Abstract** Electron impact excitation of all the  $np^5nd$ ,  $J = 0, 1, 2, 3$  and  $4$ , and  $np^5(n+2)s$ ,  $J = 0, 1$  and  $2$  states of argon ( $n = 3$ ) and xenon ( $n = 5$ ) atoms from the ground  $np^5 J = 0$  state has been considered in the fully relativistic distorted-wave approximation theory. Results for the differential cross sections are calculated in the incident electron energy range of 15 to 100 eV. The results at selected energies are only presented. These are compared with the available experimental data and where possible with the only available non-relativistic unitarized first order many body theory calculations.

**Keywords** Electron impact excitation, relativistic distorted wave approximation, differential cross sections

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### 1. Introduction

Recently considerable interest has been generated in the study of inelastic collisions of electrons with heavier atoms such as the noble gases. The choice of the noble gases is important as these are easy targets for experimentalists and provide an excellent testing ground for the theoretical models incorporating relativistic effects. Further, their electron excitation cross sections are having several useful applications *e.g.* in the study of laser and plasma physics. However, most earlier studies in the inert gases have so far mainly considered only the excitation of the lowest excited  $np^5(n+1)s$  states with  $J = 0, 1$  and  $2$  from the ground  $np^6 J = 0$  state and we now fairly well understand such excitations.

Consequently, recent activities have focused interest in studying the other higher lying  $np^5n'l$  excited states in the inert gases and more theoretical and experimental works are being reported [1, 2]. In one of our earlier papers [3] we presented detailed relativistic distorted-wave (RDW) calculations for the electron impact excitation of the  $np^6 J = 0$  state to  $np^5(n+1)p$ ,  $J = 1, 2$  and  $3$  states of Ne ( $n = 2$ ), Ar ( $n = 3$ ), Kr ( $n = 4$ ) and Xe ( $n = 5$ ). In continuation to this work we extend our RDW calculation in the present paper to similar other higher excitations *viz.*  $np^5nd$  with  $J = 0, 1, 2, 3$  and  $4$  states as well as the  $np^5(n+2)s$  with  $J = 0, 1$  and  $2$  states in the

argon ( $n = 3$ ) and xenon ( $n = 5$ ) for which we have recently completed our calculations. In fact, not much attention has been paid to study the excitation of the  $np^5 nd$   $J = 0, 1, 2, 3$ , and 4 and  $np^5 (n+2)s$   $J = 0, 1$  and 2 excited states of the inert gases. Although differential cross section (DCS) measurements for such excitations were reported much earlier for neon ( $n = 2$ ), argon ( $n = 4$ ), krypton ( $n = 5$ ) and xenon ( $n = 5$ ) but no theoretical calculations have been reported. For example the experimental DCS were reported for resolved and unresolved excitation in argon, by Chutjian and Cartwright [4] and for some of the unresolved excitations in xenon by Filipovic *et al* [5] and recently by Khakoo *et al* [2]. With their experimental data, Khakoo *et al* [2] also presented non-relativistic distorted wave approximation (DWA) and first-order many body theory (FOMBT) calculations. Therefore, for an understanding of such excitations and for comparison of the experimental differential cross section data available, there is need for a systematic theoretical investigation of the problem and also to report the reliable results.

We have carried out RDW calculations for all the excited  $np^5 nd$ ,  $J = 0, 1, 2, 3$  and 4 states and  $np^5 (n+2)s$ ,  $J = 0, 1$  and 2 states of argon ( $n = 3$ ) and xenon ( $n = 5$ ) from the  $np^6$   $J = 0$  state and report DCS results at various selected energies including those for which experimental data are available.

## 2. Theory

### 2.1 RDW theory:

We follow the RDW theory as described by Zuo *et al* [6] and discussed by us in our previous work [1, 3a, 7, 8]. In case of electron impact excitation of an atom (with  $N$  electrons) for the transition from an initial state 'a' to a final state 'b', the RDW  $T$ -matrix element is given by (atomic units are used throughout)

$$T_{b \leftarrow a} = T(J_b, M_b, \mu_b; J_a, M_a, \mu_a) = \langle \phi_b(1, \dots, N) F_{b, \mu_b}(\mathbf{k}_b, N+1) | V - U | \not\phi_a(1, \dots, N) F_{a, \mu_a}^+(\mathbf{k}_a, N+1) \rangle. \quad (1)$$

Here,  $\mathbf{k}_a$  and  $\mathbf{k}_b$  are respectively the wave vectors of the incident and scattered electrons with associated  $\mu_a$  and  $\mu_b$  as their spin projections. The quantum numbers  $J_a, J_b$  and  $M_a, M_b$  refer to the total angular momentum of the atom and its  $z$ -component respectively. Here,  $\phi_{a,b}$  are bound state wavefunctions of the target atom which are constructed from Dirac-Fock determinants obtained by solving the Dirac-Fock equations.  $F_{a,(b)}^{+(-)}$  are the projectile electron distorted waves where the plus and minus signs indicate usual outgoing and incoming asymptotic boundary conditions.  $\not\phi$  is the antisymmetrizing operator to take electron exchange into account.  $U$  is the distortion potential (which is taken as the function of only radial coordinates of the projectile electron) for obtaining the distorted projectile electron wave.  $V$  is the interaction potential between projectile electron and the target atom given by

$$V = -\frac{Z}{r_{N+1}} + \sum_{i=1}^N \frac{1}{|\mathbf{r}_i - \mathbf{r}_{N+1}|}, \quad (2)$$

$Z$  is the nuclear charge of the atom.

Following relativistic version of partial wave expansion is used for the electron distorted waves

$$F_{ch,\mu}^{\pm}(\mathbf{k}, \mathbf{r}) = \frac{1}{(2\pi)^{3/2}} \sum_{\kappa m} e^{\pm i\eta_{\kappa}} a_{\kappa m}^{\mu}(\hat{\mathbf{k}}_{ch}) \frac{1}{r} \begin{pmatrix} f_{\kappa}(r) & \chi_{\kappa m} \\ g_{\kappa}(r) & \chi_{-\kappa m} \end{pmatrix} \quad (3a)$$

with

$$a_{\kappa m}^{\mu}(\hat{\mathbf{k}}_{ch}) = 4\pi^{1/2} \left( \frac{E_{ch} + 2c^2}{2E_{ch}} \right) \sum_{m_l} \left( l m_l \frac{1}{2} \mu / j m \right) Y_{lm_l}^*(\hat{\mathbf{k}}_{ch}). \quad (3b)$$

The  $l$  and  $j$  refer respectively to the orbital and angular momentum of the projectile electron where  $ch$  and  $\mu$  denote the scattering channel and spin orientation of the channel, respectively. The radial distorted waves  $f_{\kappa}(r)$  and  $g_{\kappa}(r)$  are solutions of the following pair of integro-differential equations

$$\left( \frac{d}{dr} + \frac{\kappa}{r} \right) f_{\kappa}(r) - \frac{1}{c} (2c^2 - U + E_{ch}) g_{\kappa}(r) - \frac{1}{cr} W_Q(\kappa; r) = 0, \quad (4a)$$

$$\left( \frac{d}{dr} - \frac{\kappa}{r} \right) g_{\kappa}(r) + \frac{1}{c} (-c^2 - U + E_{ch}) f_{\kappa}(r) + \frac{1}{cr} W_P(\kappa; r) = 0, \quad (4b)$$

with the asymptotic boundary conditions

$$f_{\kappa}(r) \sim \frac{1}{\kappa_{ch}} \sin \left( \kappa_{ch} r - \frac{l\pi}{2} + \eta_{\kappa} \right), \quad (5a)$$

$$g_{\kappa}(r) \sim \frac{c}{c^2 + E_{ch}} \cos \left( \kappa_{ch} r - \frac{l\pi}{2} + \eta_{\kappa} \right). \quad (5b)$$

Here,  $W_{P,Q}$  are the non-local exchange kernels as described and discussed by McEachran and Stauffer [9]. These coupled eqs. (4a) and (4b) are solved numerically as described by Zuo *et al* [6].  $E$  is the relativistic energy of the projectile electron *i.e.*  $E_{ch} = (c^2 \kappa_{ch}^2 + c^4)^{1/2}$ . Here  $\kappa = l$  if  $j = l - 1/2$  and  $\kappa = -l - 1$  if  $j = l + 1/2$ .  $\chi_{\pm\kappa m}$  are the spin angular function and  $\eta_{\kappa}$  is the phase shift of the partial wave.

For a particular excitation, we first obtain Dirac-Fock atomic target wavefunction as described in the next section 2.2. The distortion potential  $U$  is then calculated for obtaining the projectile distorted waves by taking it as the spherically averaged static potential of the excited state as done in our previous calculations [7]. Thereafter, the  $T$ -matrix elements given by eq. (1) are first decomposed into the direct and exchange terms and then evaluated using straightforward through lengthy angular momentum algebra and carrying out numerically the involved radial integrals [6].

From the calculated  $T$ -matrix elements, the various collisional parameters can be determined. Here, we define the scattering amplitude following the normalization convention of Taylor [10] and express it as

$$f(J_b, M_b, \mu_b; J_a, M_a, \mu_a) = (2\pi)^2 \left( \frac{k_b}{k_a} \right)^{1/2} T(J_b, M_b, \mu_b; J_a, M_a, \mu_a) \quad (6)$$

Further, for a given value of  $J_b$  and  $J_a$ , the DCS for an unpolarized electron beam scattering from an unpolarized atom is defined as

$$\sigma = \sum \langle f(M'_b) f^*(M_b) \rangle, \quad (7)$$

where the angle brackets imply an average over all the initial atomic and spin states and sum over the final spin state *i.e.*

$$\begin{aligned} \langle f(M'_b) f^*(M_b) \rangle &= \frac{1}{2(2J_a + 1)} \sum_{M_a \mu_a \mu_b} f(J_b, M'_b, \mu_b; J_a, M_a, \mu_a) \\ &\times f^*(J_b, M_b, \mu_b; J_a, M_a, \mu_a). \end{aligned} \quad (8)$$

In this expression, we have suppressed the notations  $J_a$ ,  $J_b$ , and  $M_a$ .

## 2.2 Target wavefunctions :

In the relativistic atomic structure description of Grant [11], the configuration of the ground state can be represented as  $n\bar{p}^2 np^4$  and the excited states by  $n\bar{p}np^4mj$  or  $np^2 np^3mj$ . Here, all the inner subshells ( $1s$ - $ns$ ) are full and therefore not specified. Also the excited  $mj$  orbital can be either  $n\bar{d}$  or  $nd$  or  $(n+2)s$  in the present context. The transitions which are considered in the present work will arise due to the excitation of one outer electron from the ground state orbital  $n\bar{p}$  or  $np$  to either  $n\bar{d}$  or  $nd$  and  $(n+2)s$  orbitals. Thus, we can represent the states of interest in this paper by the outer three subshells alongwith the  $J$  value representing the total angular momentum of the atom. The ground state of these two noble gases is given by

$$\phi_a = (n\bar{p}^2 np^4)_{J_a=0} \quad (9)$$

and the excited states with excitation to a  $\bar{d}$  or  $d$  orbital for different  $J_b$  are

$$\phi_b(J_b = 0) = - (n\bar{p}np^3 m\bar{d})_{J_b=0}, \quad (10a)$$

$$\phi_b(J_b = 1) = C_1 (n\bar{p}^2 np^3 m\bar{d})_{J_b=1} + C_2 (n\bar{p}^2 np^3 md)_{J_b=1} + C_3 (n\bar{p}np^4 m\bar{d})_{J_b=1}, \quad (10b)$$

$$\begin{aligned} \phi_b(J_b = 2) &= C_1 (n\bar{p}^2 np^3 m\bar{d})_{J_b=2} + C_2 (n\bar{p}np^3 md)_{J_b=2} \\ &+ C_3 (n\bar{p}np^4 m\bar{d})_{J_b=2} + C_4 (npnp^4 md)_{J_b=2}, \end{aligned} \quad (10c)$$

$$\phi_b(J_b = 3) = C_1 (n\bar{p}^2 np^3 m\bar{d})_{J_b=3} + C_2 (n\bar{p}^2 np^3 md)_{J_b=3} + C_4 (n\bar{p}np^4 md)_{J_b=3} \quad (10d)$$

and

$$\phi_b(J_b = 4) = (np^2 np^3 md)_{J_b=4}. \quad (10e)$$

Here, we will take for present case  $m = n$ . In terms of intermediate coupling scheme there are three excited states for  $J_b = 1$  i.e.  $md [1/2]_1$ ,  $md [3/2]_1$ ,  $md' [3/2]_1$ , four excited states for  $J_b = 2$  i.e.  $md [3/2]_2$ ,  $md [5/2]_2$ ,  $md' [5/2]_2$  and  $md' [3/2]_2$ , three excited states for  $J_b = 3$  i.e.  $md [7/2]_3$ ,  $md [5/2]_3$ ,  $md' [5/2]_3$  and only one each for  $J_b = 0$  and 4 i.e.  $md [1/2]_0$  and  $md [7/2]_4$  with different values of configuration mixing coefficients  $C_1$ ,  $C_2$ ,  $C_3$  and  $C_4$  for Ar ( $m = 3$ ) and Xe ( $m = 5$ ) as given in Table 1. The radial wavefunctions of the different orbitals and the corresponding configuration mixing coefficients are obtained using relativistic multiconfiguration Dirac-Fock (MCDF) program of Grant *et al* [12].

**Table 1.** Values of the configuration mixing coefficients  $C_1$ ,  $C_2$ ,  $C_3$  and  $C_4$  corresponding to the different excited states  $np^5nd$ ,  $J_b = 1, 2$  and 3 of Ar and Xe as used in equations (10)

Atom	$J_b$	Excited State	$C_1$	$C_2$	$C_3$	$C_4$
Argon ( $n = 3$ )	1	3d $[1/2]_1$	-0.80877337	0.55079335	-0.20618515	
		3d $[3/2]_1$	0.58597484	0.72475936	-0.36243256	
		3d' $[3/2]_1$	0.05019083	0.41394512	0.90891711	
	2	3d $[3/2]_2$	-0.38859345	0.86125254	-0.06431457	0.32109628
		3d $[5/2]_2$	-0.87110448	-0.39327622	0.28827557	0.05837803
		3d' $[5/2]_2$	0.25855365	0.14045215	0.94739762	0.12594028
		3d' $[3/2]_2$	0.15771582	-0.28957048	0.12328253	0.93681814
	3	3d $[7/2]_3$	0.98968022	0.04794930		0.13503308
		3d $[5/2]_3$	0.02455101	-0.98515815		0.16988429
		3d' $[5/2]_3$	-0.14117477	0.16481592		0.97616873
Xenon ( $n=5$ )	1	5d $[1/2]_1$	0.85256869	-0.51182254	0.10566129	
		5d $[3/2]_1$	0.52224079	0.82671260	-0.20931036	
		5d' $[3/2]_1$	-0.01977824	-0.23363209	-0.97212389	
	2	5d $[3/2]_2$	-0.40085672	0.90710708	-0.02538691	0.1258020
		5d $[5/2]_2$	0.91096954	0.40286412	-0.08632121	-0.0195868
		5d' $[5/2]_2$	-0.06258857	0.11176137	0.08528474	-0.9880884
		5d' $[3/2]_2$	-0.07437106	-0.04864812	-0.99228558	-0.0864387
	3	5d $[7/2]_3$	0.99814718	0.00020509		0.0608454
		5d $[5/2]_3$	0.00222538	0.99920221		-0.0398747
		5d' $[5/2]_3$	-0.06080500	0.0399362		0.9973504

Similarly, the excited states with excitation to a  $s$  orbital for different  $J_h$  are :

$$\hat{\psi}_h(J_h = 0) = - \left( n\bar{p}np^4ms \right)_{J_h=0} \quad (11a)$$

$$\phi_h(J_h = 1) = C_1 \left( n\bar{p}np^4ms \right)_{J_h=1} + C_2 \left( n\bar{p}^2np^3ms \right)_{J_h=1} \quad (11b)$$

and

$$\phi_h(J_h = 2) = - \left( n\bar{p}^2np^3ms \right)_{J_h=2} \quad (11c)$$

There are thus two excited states for  $J_h = 1$  i.e.  $ms [3/2]_1$  and  $ms' [1/2]_1$  and only one excited state for  $J_h = 0$  and 2 i.e.  $ms' [1/2]_0$  and  $ms [3/2]_2$ . The different values of configuration mixing coefficients  $C_1$  and  $C_2$  for Ar ( $m = 5$ ) and Xe ( $m = 7$ ) are given in Table 2.

**Table 2.** Values of the configuration mixing coefficients  $C_1$ ,  $C_2$ ,  $C_3$  and  $C_4$  corresponding to the different excited states  $np^5(n+2)s$ ,  $J_h = 1$  of Ar and Xe as used in eqs (11)

Atom	$J_h$	Excited State	$C_1$	$C_2$
Argon ( $n=3$ )	1	5s $[3/2]_1$	0.01250588	0.99214934
		5s' $[1/2]_1$	-0.99214934	0.01250588
Xenon ( $n = 5$ )	1	7s $[3/2]_1$	0.01594722	0.99987284
		7s' $[1/2]_1$	-0.99987284	0.01594722

### 3. Results and discussion

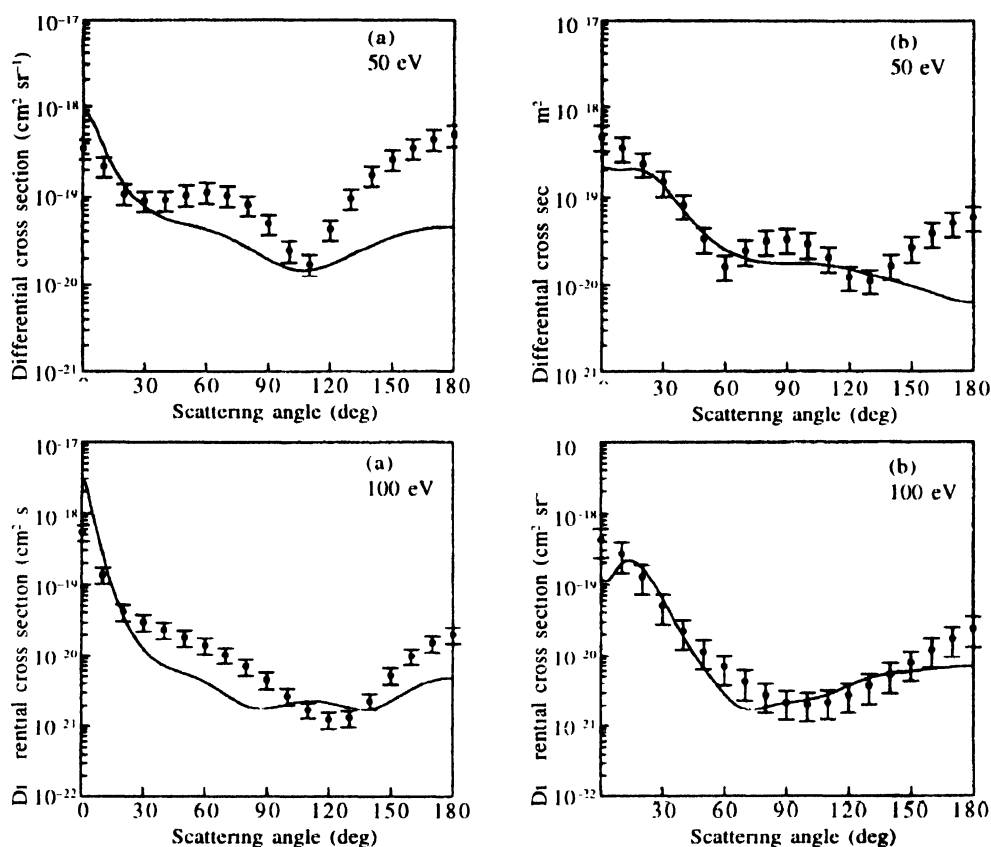
As we explained in our earlier paper [3b] for both the  $np^5nd$  and  $np^5(n+1)s$ , the excitations for the various allowed odd values of  $J_h$  i.e. the states with  $J_h = 1$  or 3 can occur *via* a direct interaction as well as *via* exchange while for states with even values of  $J_h = 0, 2$  and 4 the excitation can occur only *via* exchange. The DCS for direct excitations are characterized by strong forward peak and generally having larger values than those for exchange transitions. The theoretical cross sections for the exchange transitions are relatively flat in the forward direction. We discuss below our various results alongwith comparison with other available data.

#### 3.1 Argon :

Present RDW results for the DCS of the argon atom are compared in the Figures 1-3 with the experimental data of Chutjian and Cartwright [4]. They measured the DCS in the angular range  $5-138^\circ$  and then extrapolated these results to both forward and backward scattering angles. Also, they put their DCS data on an absolute scale with respect to their earlier elastic scattering measurements. No theoretical results are available for comparison.

In Figures 1 we present RDW DCS results for the unresolved  $3d [1/2]_0 + 3d [1/2]_1$  states and  $3d [7/2]_3$  state at 50 and 100 eV. The agreement of our RDW results with the experiment is

quite good except for the extrapolated experimental values at the near forward and backward scattering angles.



**Figure 1.** Comparison of the differential cross sections (in units of  $\text{cm}^2 \text{sr}^{-1}$ ) for excitation of (a) the unresolved  $3d [1/2]_0 + 3d [1/2]_1$  and (b)  $3d [7/2]_1$  at 50 and 100 eV in argon

— Present RDW results,

••••• Experimental data of Chutjian and Cartwright (1981)

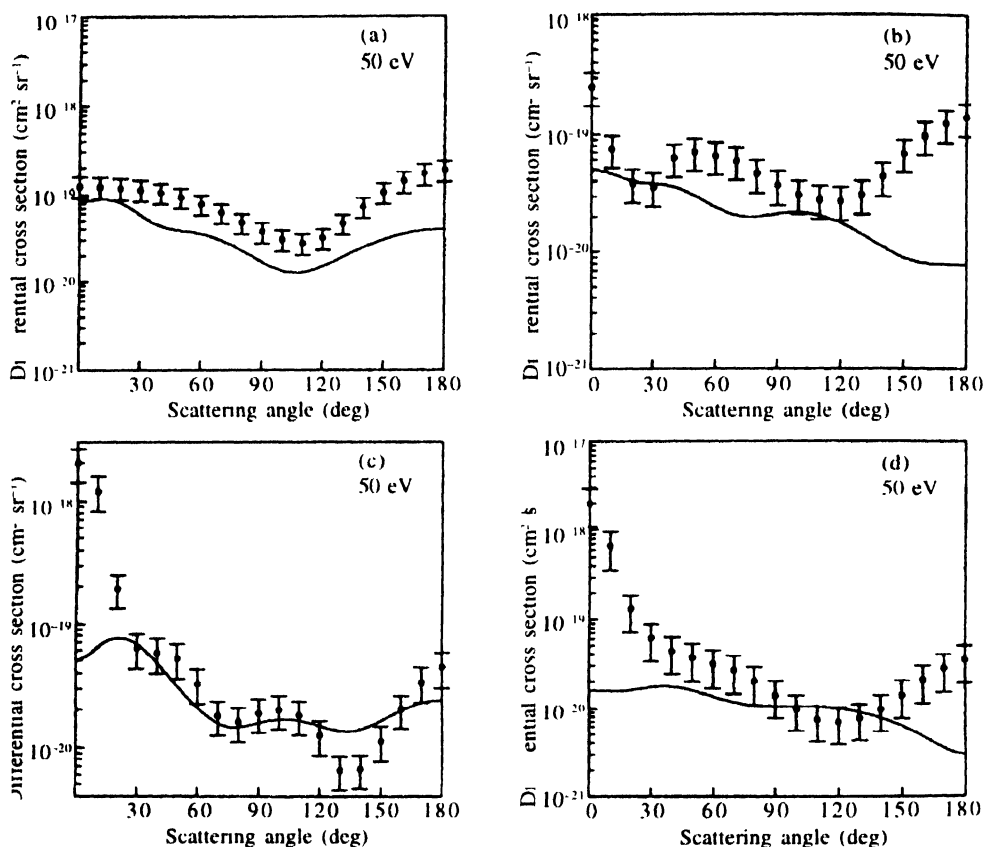
Figures 2(a) to 2(d) contain the DCS results for the  $3d [3/2]_2$ ,  $3d [7/2]_4$ , the unresolved  $3d [5/2]_2 + 5s [3/2]_2$  and  $3d' [5/2]_2$  states, respectively at 50 eV. As expected the cross sections are relatively flat and the agreement is less satisfactory as excitations to these states are *via* exchange [3b].

In Figures 3(a) to 3(d), the DCS results are compared at 100 eV for the unresolved  $5s [3/2]_1 + 3d [5/2]_3$ ,  $3d [3/2]_1$ ,  $3d' [3/2]_1$  states and the unresolved  $3d' [3/2]_2 + 3d' [5/2]_3 + 5s' [1/2]_0 + 5s' [1/2]_1$  at 50 eV. These cross sections have the strong forward peak and agree very well in shape and magnitude in this angular range with experiment.

### 3.2 Xenon :

In Figures 4 and 5 we show the DCS results for the excitations of the different  $5p^55d$ ,  $J_b = 1, 2$  and 3 as well as  $5p^57s$ ,  $J_b = 1$  and 2 states of xenon. The experimental data for these excitations are available for the  $5d [3/2]_1$ ,  $5d [5/2]_2$ ,  $5d [5/2]_3$ ,  $5d [7/2]_3$  and the unresolved  $7s [3/2]_2 + 7s [3/2]_1$

states at 15, 20 and 30 eV in the angular range 0 to  $135^\circ$  from Khakoo *et al* [2] and in the range of 0 to  $150^\circ$  from Filipovic' *et al* [5]. They measured the relative DCS values and put them on absolute scale, with respect to the combined first two lowest excited states of xenon, which in



**Figure 2.** Same as in Figure 1 but for (a)  $3d [3/2]_2$ , (b)  $3d [7/2]_4$ , (c)  $3d [5/2]_2 + 5s [3/2]_2$ , and (d)  $3d' [5/2]_2$ , at 50 eV in argon

turn were normalized with the help of the elastic DCS measurements of Register *et al* [13]. Khakoo *et al* [2] also reported the non-relativistic DWA and FOMBT calculations and found the later to be the more reliable. We have included only their FOMBT calculations in our comparisons. Further, Filipovic' *et al* [5] have also reported experimental DCS for  $5d [3/2]_1$  state at 80 eV while Khakoo *et al* [2] did not report any experimental measurements for DCS of  $5d [3/2]_1$  state at 80 eV. However, Khakoo *et al* [2] compared their theoretical non-relativistic DWA and FOMBT calculations with the data of Filipovic' *et al* [5].

In Figures 4(a) to 4(d), we present the DCS results respectively for xenon at 30 eV, for  $5d [7/2]_3$ ,  $5d [5/2]_3$  and  $5d [3/2]_1$  states as well as 80 eV for  $5d [3/2]_1$ . The cross sections for  $5d [7/2]_3$  and  $5d [5/2]_3$  states do not show forward peaking as in case of  $5d [3/2]_1$  state. The agreement with the experiment is good and the RDW results and FOMBT results of Khakoo *et al* [2] have similar behavior. For  $5d [7/2]_3$  and  $5d [5/2]_3$  states at 30 eV the RDW results are in better qualitative agreement with the experiment of Khakoo *et al* [2] and for  $5d [3/2]_1$  at 80 eV, with the experiment of Filipovic' *et al* [5]



In Figures 5(a) and 5(b) the RDW results for the  $5d [5/2]_2$  and the unresolved  $7s [3/2]_2 + 7s [3/2]_1$  states at 30 eV are shown. The excitation to  $5d [5/2]_2$  state is an exchange transition and thus obviously has a relatively flat DCS and the agreement with experiment is less satisfactory. The agreement with the experiment for the unresolved  $7s [3/2]_2 + 7s [3/2]_1$  states is very good.

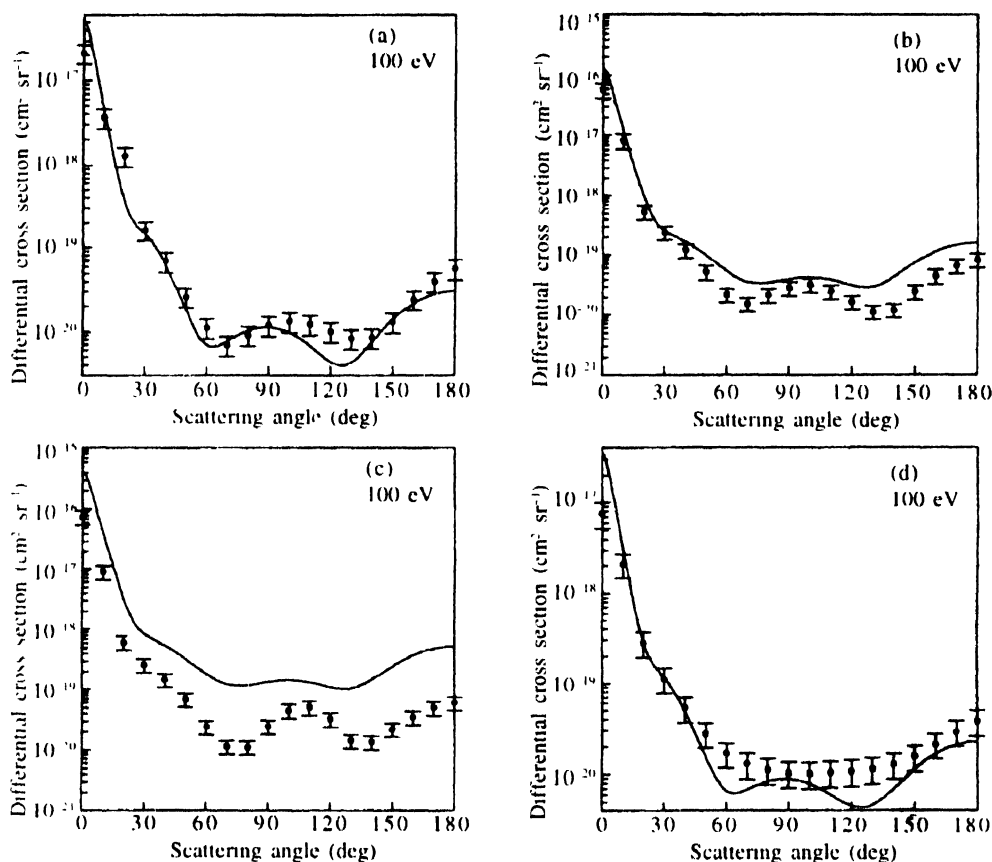


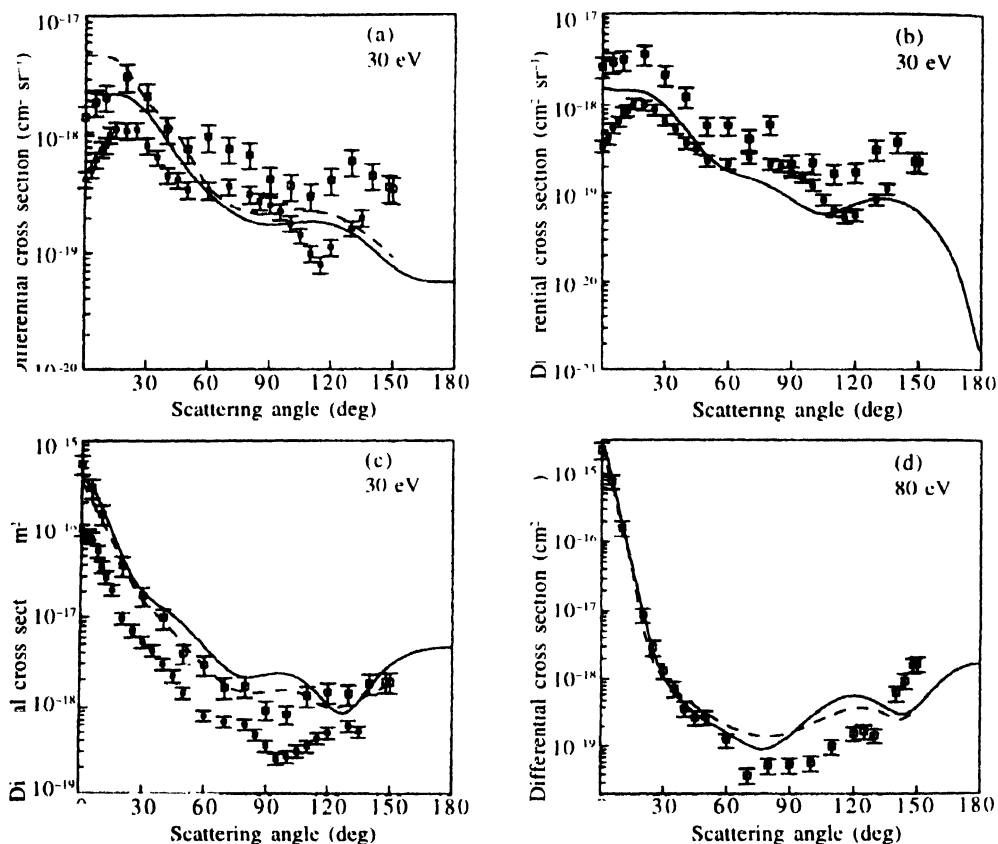
Figure 3. Same as in Figure 1 but for (a)  $5s [3/2]_1 + 3d [5/2]_1$ , (b)  $3d [3/2]_1$ , (c)  $3d' [3/2]_1$  and (d)  $3d' [3/2]_2 + 3d' [5/2]_1 + 5s' [1/2]_0 + 5s' [1/2]_1$ , at 100 eV in argon

#### 4. Conclusions

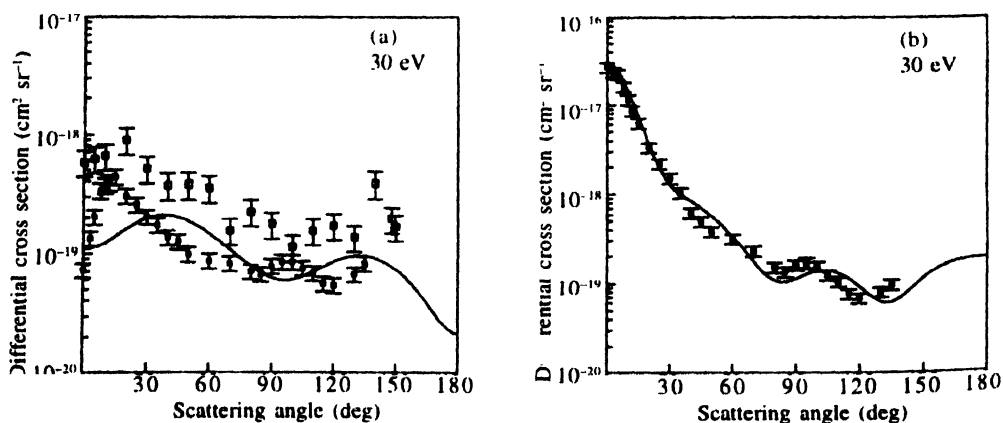
We have presented results for the excitation of  $np^5nd$ ,  $J = 0, 1, 2, 3$  and  $4$  and  $np^5(n+2)s$ ,  $J = 0, 1$  and  $2$  states of Ar ( $n = 3$ ) and Xe ( $n = 5$ ) from the ground  $np^6 J = 0$  state. There is quite good agreement between our results and the experimentally measured cross sections. To our knowledge, these represent the first reported theoretical DCS for argon for these states.

The present work confirms further the efficacy of the RDW method for electron scattering by heavy closed shell atoms. The RDW method, is a first-order theory and is expected to produce reliable results for direct excitations at higher energies and less reliable results of excitations which proceed purely *via* exchange interaction. The calculations performed are

fully relativistic, as we use Dirac-Fock wavefunctions for the bound states which are based on the  $j-j$  coupling scheme and produce distinct energy values for various fine-structure levels of the atom. Further, as can be seen, the DCS for direct excitations are characterized by strong



**Figure 4.** Same as in Figure 1 but for (a)  $5d [7/2]_1$  at 30 eV (b)  $5d [5/2]_1$  at 30 eV (c)  $5d [3/2]_2$  at 30 eV and (d)  $5d [3/2]_1$  at 80 eV in xenon. Theory, —, Present RDW results, ---, FOMBT results of Khakoo *et al* [2]; Experiment, ■, Khakoo *et al* [2], □, Filipovic *et al* [5].



**Figure 5.** Same as in Figure 4 but for (a)  $5d [5/2]_2$ , (b)  $7s [3/2]_2 + 7s [3/2]_1$  at 30 eV in xenon

forward peak and generally larger values than those for exchange transitions. Note that our RDW results for these excitations for other inert gases viz. Ne and Kr will be reported elsewhere once we have completed our calculations.

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